$(AGN)^2$

Week 1
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Selection Rules

- **Selection Rules**

(1) one electron jumps
(2) Δn any
(3) $\Delta l = \pm 1$
(4) parity change

→ selection rule for configuration

(5) $\Delta S = 0$ → ***intercombination*** line if only this rule is violated.

(6) $\Delta L = 0, \ \pm 1$ (except $L = 0 - 0$)
(7) $\Delta J = 0, \ \pm 1$ (except $J = 0 - 0$)
(8) $\Delta F = 0, \ \pm 1$ (except $F = 0 - 0$) → It is only rarely necessary to consider this.

- ***Allowed = Electric Dipole*** : Transitions which satisfy all the above selection rules are referred to as ***allowed transitions***. These transitions are strong and have a typical lifetime of $\sim 10^{-8}$ s. Allowed transitions are denoted without square brackets.

$$\text{e.g., C IV } 1548, 1550 \text{ Å}$$

- Photons do not change spin, so transitions usually occur between terms with the same spin state ($\Delta S = 0$). However, relativistic effects mix spin states, particularly for high *Z* atoms and ions. As a result, one can get (weak) spin changing transitions. These are called ***intercombination (semi-forbidden or intersystem) transitions*** or lines. They have a typical lifetime of $\sim 10^{-3}$ s. An intercombination transition is denoted with a single right bracket.

$$\text{C III] } 2s^2\ {}^1S - 2s2p\ {}^3P^o \text{ at } 1908.7\,\text{Å}. \quad (\Delta S = 1)$$

- If any one of the rules 1-4, 6-8 are violated, they are called ***forbidden transitions*** or lines. They have a typical lifetime of $\sim 1 - 10^3$ s. A forbidden transition is denoted with two square brackets.

$$1906.7\,\text{Å [C III] } 2s^2\ {}^1S_0 - 2s2p\ {}^3P^o_2, \quad (\Delta S = 1, \Delta J = 2)$$

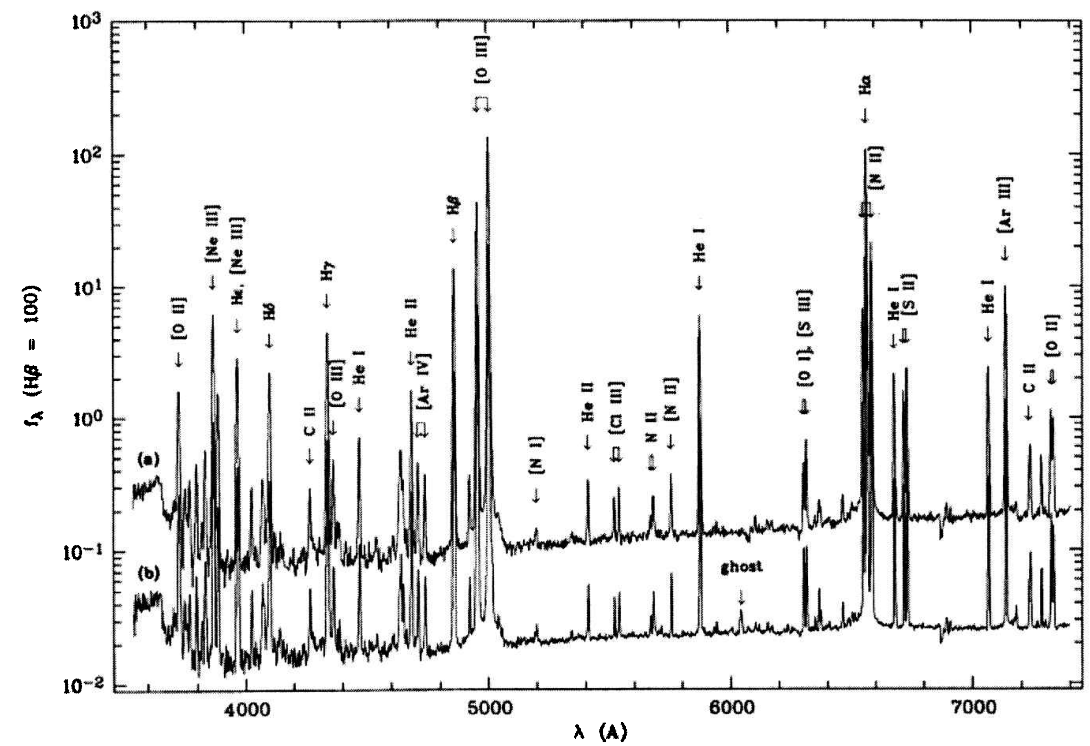
- ***Resonance line*** denotes the longest wavelength, dipole-allowed transition arising from the ground state of a particular atom or ion.

Forbidden Lines

- Forbidden lines are often difficult to study in the laboratory as collision-free conditions are needed to observe metastable states.
  - In this context, it must be remembered that laboratory ultrahigh vacuums are significantly denser than so-called dense interstellar molecular clouds.
  - ***Even in the best vacuum on Earth, frequent collisions knock the electrons out of these orbits (metastable states) before they have a chance to emit the forbidden lines.***
  - In astrophysics, low density environments are common. In these environments, the time between collisions is very long and an atom in an excited state has enough time to radiate even when it is metastable.
  - Forbidden lines of nitrogen ([N II] at 654.8 and 658.4 nm), sulfur ([S II] at 671.6 and 673.1 nm), and oxygen ([O II] at 372.7 nm, and [O III] at 495.9 and 500.7 nm) are commonly observed in astrophysical plasmas. ***These lines are important to the energy balance of planetary nebulae and H II regions.***
  - ***The forbidden 21-cm hydrogen line is particularly important for radio astronomy as it allows very cold neutral hydrogen gas to be seen.***
  - Since metastable states are rather common, forbidden transitions account for a significant percentage of the photons emitted by the ultra-low density gas in Universe.
  - ***Forbidden lines can account for up to 90% of the total visual brightness of objects such as emission nebulae.***

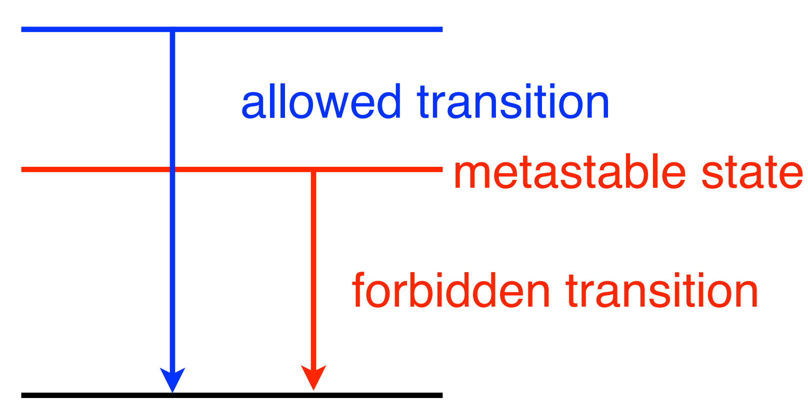
History: Nebulium?

- In 1918, extensive studies of the emission spectra of nebulae found a series of lines which had not been observed in the laboratory.
  - Particularly strong were features at 4959Å and 5007Å. For a long time, this pair could not be identified and these lines were attributed to a new element, ***'nebulium'***.
  - In 1927, Ira Bowen (1898-1973) discovered that the lines were not really due to a new chemical element but instead ***forbidden lines from doubly ionized oxygen*** [O III].
  - He realized that in the diffuse conditions found in nebulae, atoms and ions could survive a long time without undergoing collisions. Indeed, ***under typical nebula conditions the mean time between collisions is in the range 10-10,000 secs.*** This means that there is sufficient time for excited, metastable states to decay via weak, forbidden line emissions.
  - The forbidden lines could not be observed in the laboratory where it was not possible to produce collision-free conditions over this long timeframe.
  - Other 'nebulium' lines turned out to be forbidden lines originating from singly ionized oxygen [O II] and nitrogen [N II].



Optical spectra of NGC 6153, Liu et al. (2000, MNRAS)

[O III], [O II], [N II], etc:
We use a pair of square brackets for a forbidden line.



Notations

- Notations for Spectral Emission Lines and for Ions
  - There is a considerable confusion about the difference between these two ways of referring to a spectrum or ion, for example, C III or C^{+2}. These have very definite different physical meanings. However, in many cases, they are used interchangeably.
  - C^{+2} is a baryon and C III is a set of photons.
  - C^{+2} refers to carbon with two electrons removed, so that is doubly ionized, with a net charge of +2.
  - C III is the spectrum produced by carbon with two electrons removed. The C III spectrum will be produced by impact excitation of C^{+2} or by recombination of C^{+3}. So, depending on how the spectrum is formed. C III may be emitted by C^{+2} or C^{+3}.

collisional excitation: $C^{+2} + e^- \;\rightarrow\; C^{+2*} + e^- \;\rightarrow\; C^{+2} + e^- + h\nu$

recombination: $C^{+3} + e^- \;\rightarrow\; C^{+2} + h\nu$

  - There is no ambiguity in absorption line studies - only C^{+2} can produce a C III absorption line. This had caused many people to think that C III refers to the matter rather than the spectrum.
  - But this notation is ambiguous in the case of emission lines.

- Radio Recombination Lines
  - Astronomers label each recombination line using the name of the element, the **lower level number n**, and successive letters in the Greek alphabet to denote the level change Δn.
  - α for $\Delta n = 1$, β for $\Delta n = 2$, γ for $\Delta n = 3$, etc.
  - The recombination line produced by the transition between the $n = 92$ and $n = 91$ levels of a hydrogen atom is called the $\mathrm{H}91\alpha$ line.

[Hydrogen Atom] : Fine Structure

- The discussion on H-atom levels has assumed that all states with the same principal quantum number, n, have the same energy.
  - However, this is not correct: inclusion of relativistic (or magnetic) effects split these levels according to the total angular momentum quantum number J. ***The splitting is called fine structure.***

- For hydrogen, $S = \frac{1}{2} \quad \rightarrow \quad J = L \pm \frac{1}{2}$

- Spectroscopic notation: $^{(2S+1)}L_J$

configuration	L	S	J	term	level
ns	0	$1/2$	$1/2$	^2S	$^2S_{1/2}$
np	1	$1/2$	$1/2,\ 3/2$	$^2P^o$	$^2P^o_{1/2},\ ^2P^o_{3/2}$
nd	2	$1/2$	$3/2,\ 5/2$	^2D	$^2D_{3/2},\ ^2D_{5/2}$
nf	3	$1/2$	$5/2,\ 7/2$	$^2F^o$	$^2F^o_{5/2},\ ^2F^o_{7/2}$

Note that the levels are called to be

singlet if 2S+1 = 1 $\quad S = 0, \quad J = L$

doublet if 2S+1 = 2 $\quad S = 1/2, \quad J = L \pm 1/2$

triplet if 2S+1 = 3 $\quad S = 1, \quad J = L - 1, L, L + 1$

(when L > 0)

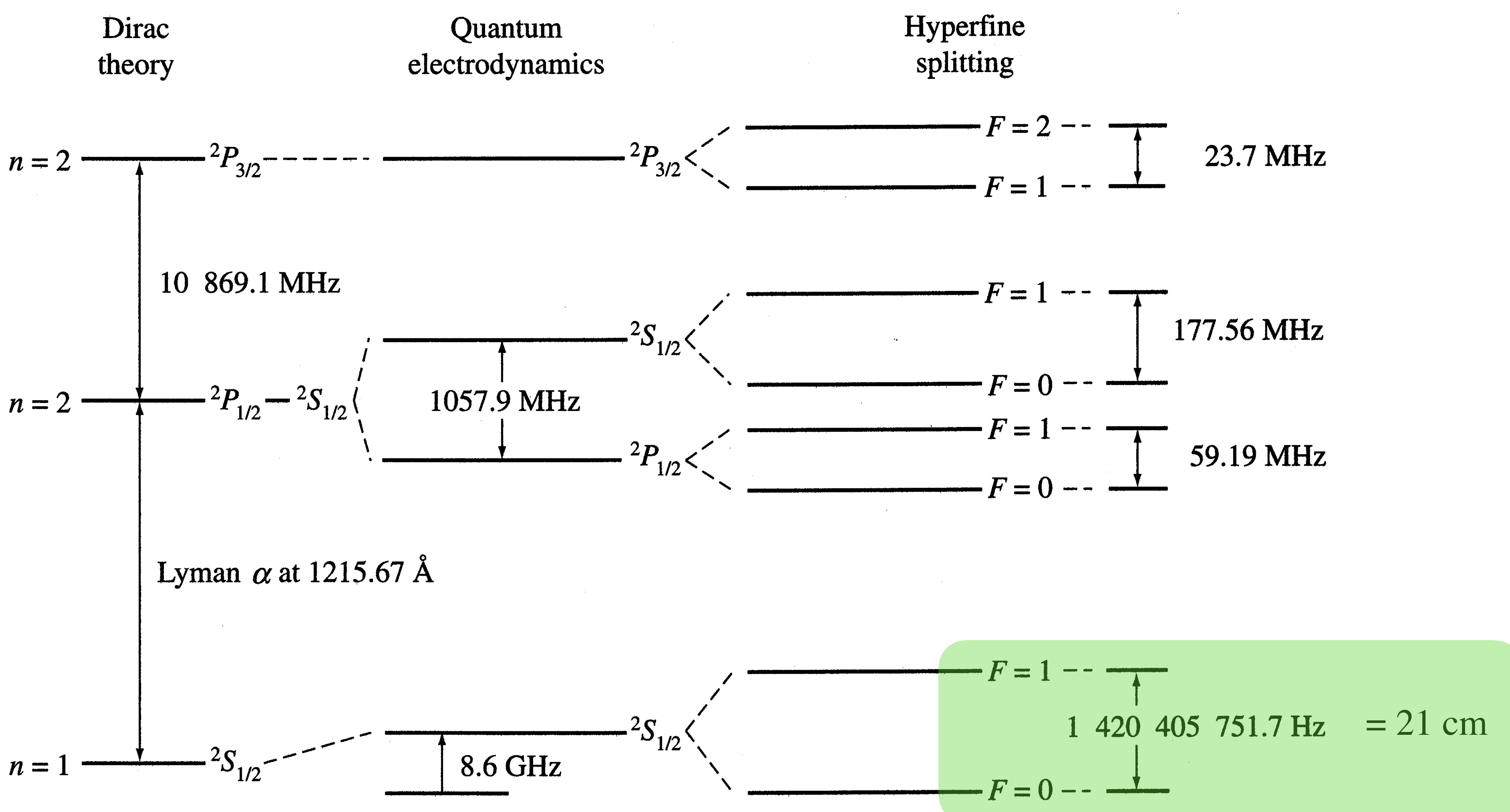
- The above table shows the fine structure levels of the H atom.
- Note that the states with principal quantum number $n = 2$ give rise to three fine-structure levels. In spectroscopic notation, these levels are $2^2S_{1/2}$, $2^2P^o_{1/2}$ and $2^2P^o_{3/2}$.

Hydrogen Atom : Hyperfine Structure

- <u>Hyperfine Structure in the H atom</u>

Coupling the nuclear spin I to the total electron angular momentum J gives the final angular momentum F. For hydrogen this means

$$F = J + I = J \pm \frac{1}{2}$$



[Kwok] Physics and Chemistry of the ISM
[Bernath] Spectra of atoms and Molecules

Hydrogen Atom : Allowed Transitions

- **Selection Rules**
  - Transitions are governed by selection rules which determine whether they can occur.

Δn any

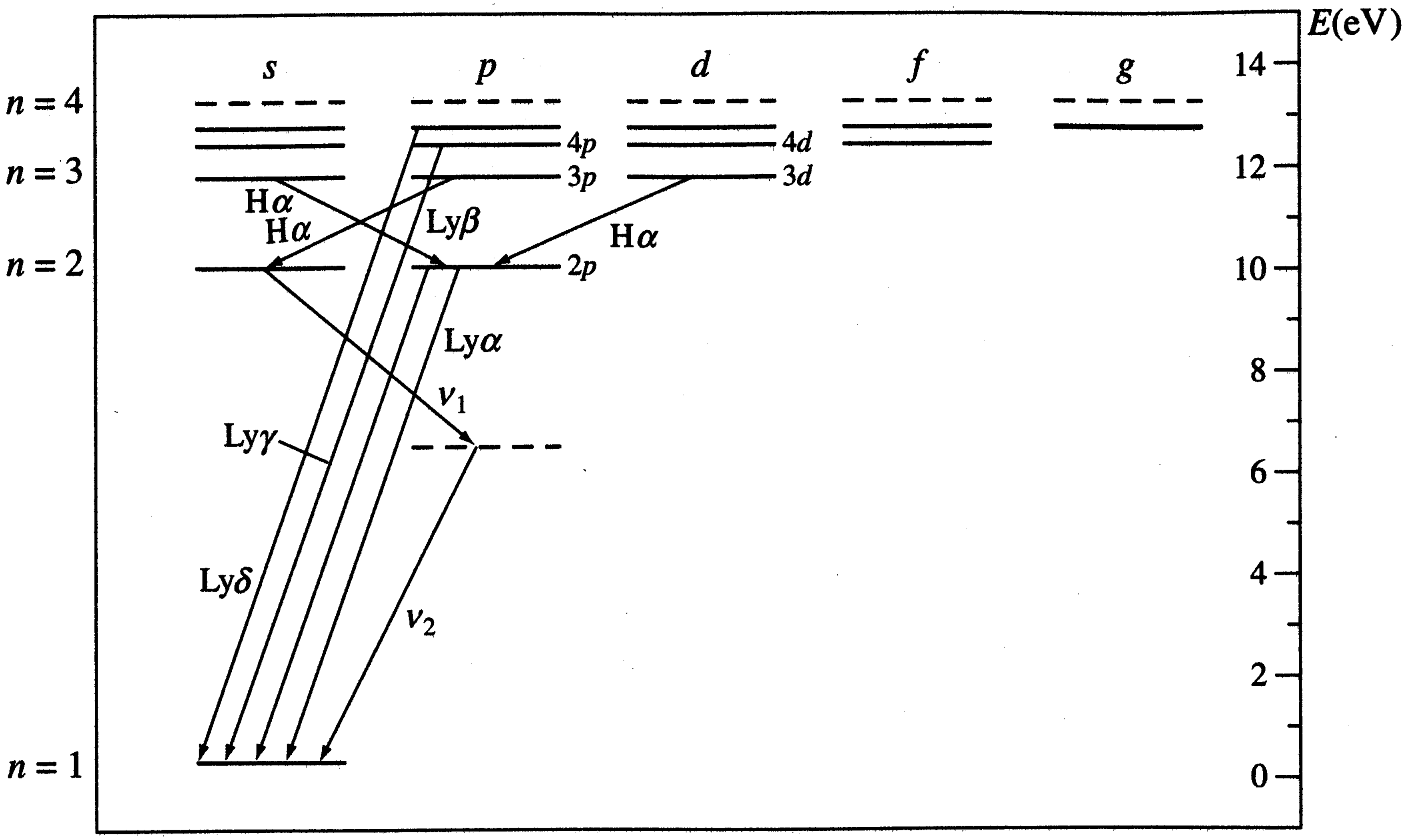
$\Delta l = \pm 1$ → selection rule for configuration

$\Delta S = 0$ → For H atom, this is always satisfied as $S = 1/2$ for all states.

$\Delta L = 0, \ \pm 1$ (not $L = 0 - 0$)

$\Delta J = 0, \ \pm 1$ (not $J = 0 - 0$)

For H-atom, l and L are equivalent since there is only one electron.



For Hα transitions:

Not all Hα transitions which correspond to $n = 2 - 3$ are allowed.

$2s_{\frac{1}{2}} - 3p_{\frac{1}{2}}$ is allowed;

$- 3p_{\frac{3}{2}}$ is allowed;

$2p_{\frac{1}{2}} - 3d_{\frac{5}{2}}$ is not allowed; ($\Delta J = 2$)

$- 3s_{\frac{1}{2}}$ is allowed;

$- 3d_{\frac{3}{2}}$ is allowed;

$2p_{\frac{3}{2}} - 3s_{\frac{1}{2}}$ is allowed;

$- 3d_{\frac{3}{2}}$ is allowed;

$- 3d_{\frac{5}{2}}$ is allowed .

The transition between $2s - 1s$ is not allowed ($\Delta l = 0$).

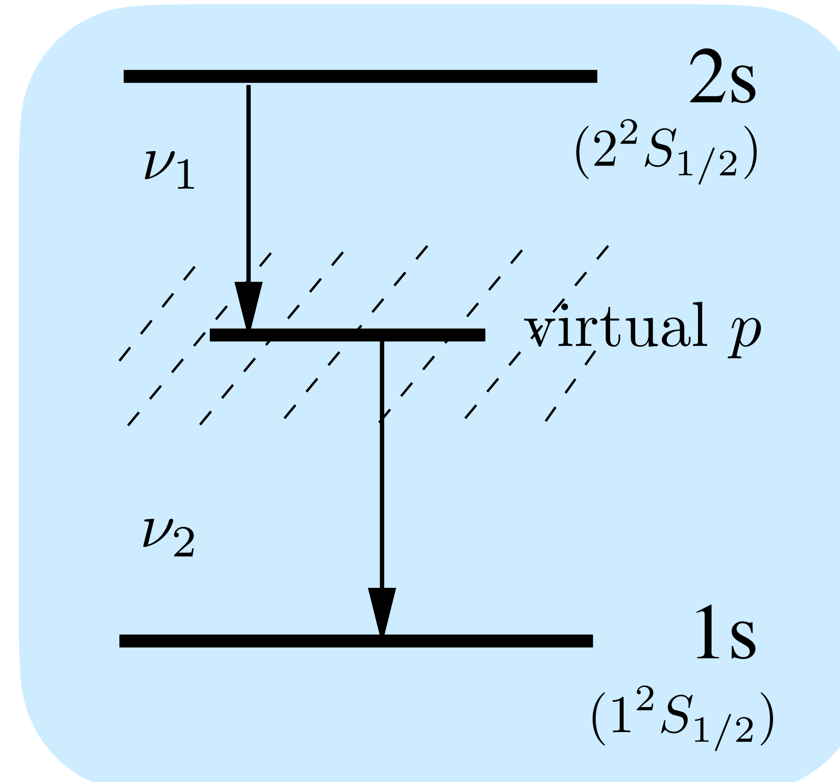
- Hydrogen: ***lifetime of excited states***

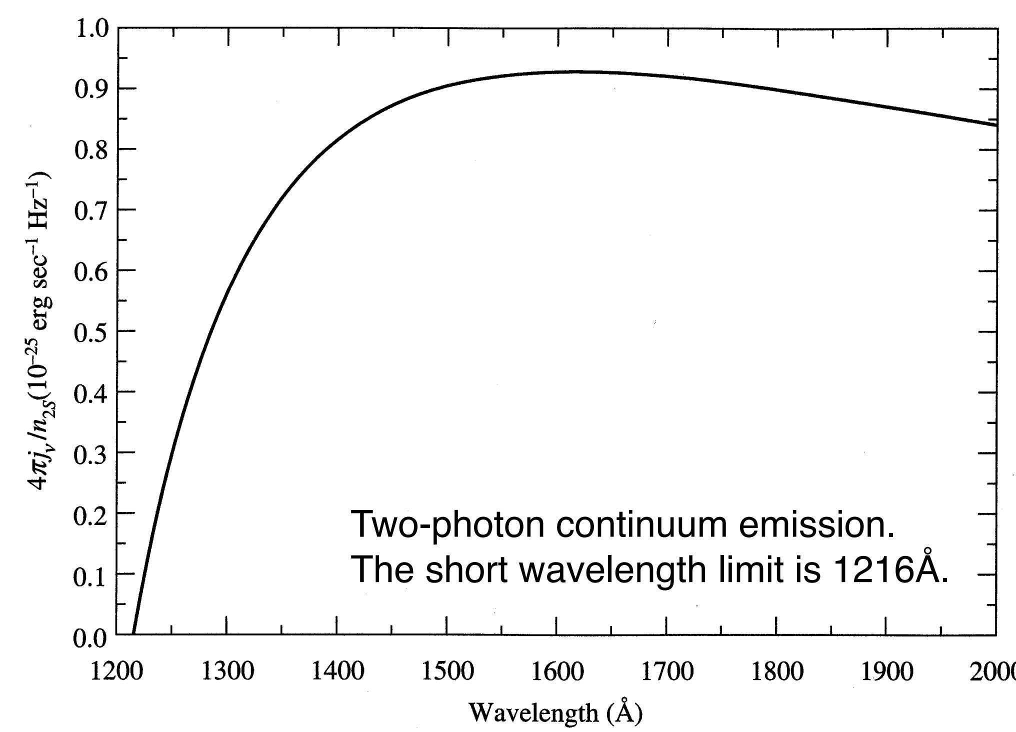
$$\tau_i = \left(\sum_j A_{ij}\right)^{-1} \quad \text{where } A_{ij} \text{ is the Einstein A coefficient}$$

Level	2s	2p	3s	3p	3d
τ/s	0.14	1.6×10^{-9}	1.6×10^{-7}	5.4×10^{-9}	2.3×10^{-7}

  - Lifetimes for allowed transitions are short, a few times 10^{-9} s.
  - However, the lifetime for the (2s) $2^2S_{1/2}$ level is ~ 0.14 s, which is 10^8 times longer than the 2p states. ***(The level is called to be metastable.)***

- ***Two-photon continuum radiation***
  - In low-density environments (e.g., ISM), an electron in the $2^2S_{1/2}$ level can jumps to a virtual *p* state, which lies between $n = 1$ and $n = 2$ levels. The electron then jumps from this virtual state to the ground state, in the process emitting two photons with total frequency $\nu_1 + \nu_2 = \nu_{\mathrm{Ly}\alpha}$.
  - Since this virtual *p* state can occur anywhere between $n = 1$ and $n = 2$, continuum emission longward of Lyα will result.
  - Because the radiative lifetime of the 2s level is long. we need to consider the possibility for collisions with electrons and protons to depopulate 2s level before a spontaneous decay occurs. However, the critical density, at which deexcitation by electron and proton collision is equal to the radiative decay rate, is $n_{\mathrm{crit}} \approx 1880\ \mathrm{cm}^{-3}$. In the ISM, the radiative decay is in general faster than the collisional depopulation process.





Ionization Potentials (eV)

[Draine] Physics of the Interstellar and Intergalactic Medium

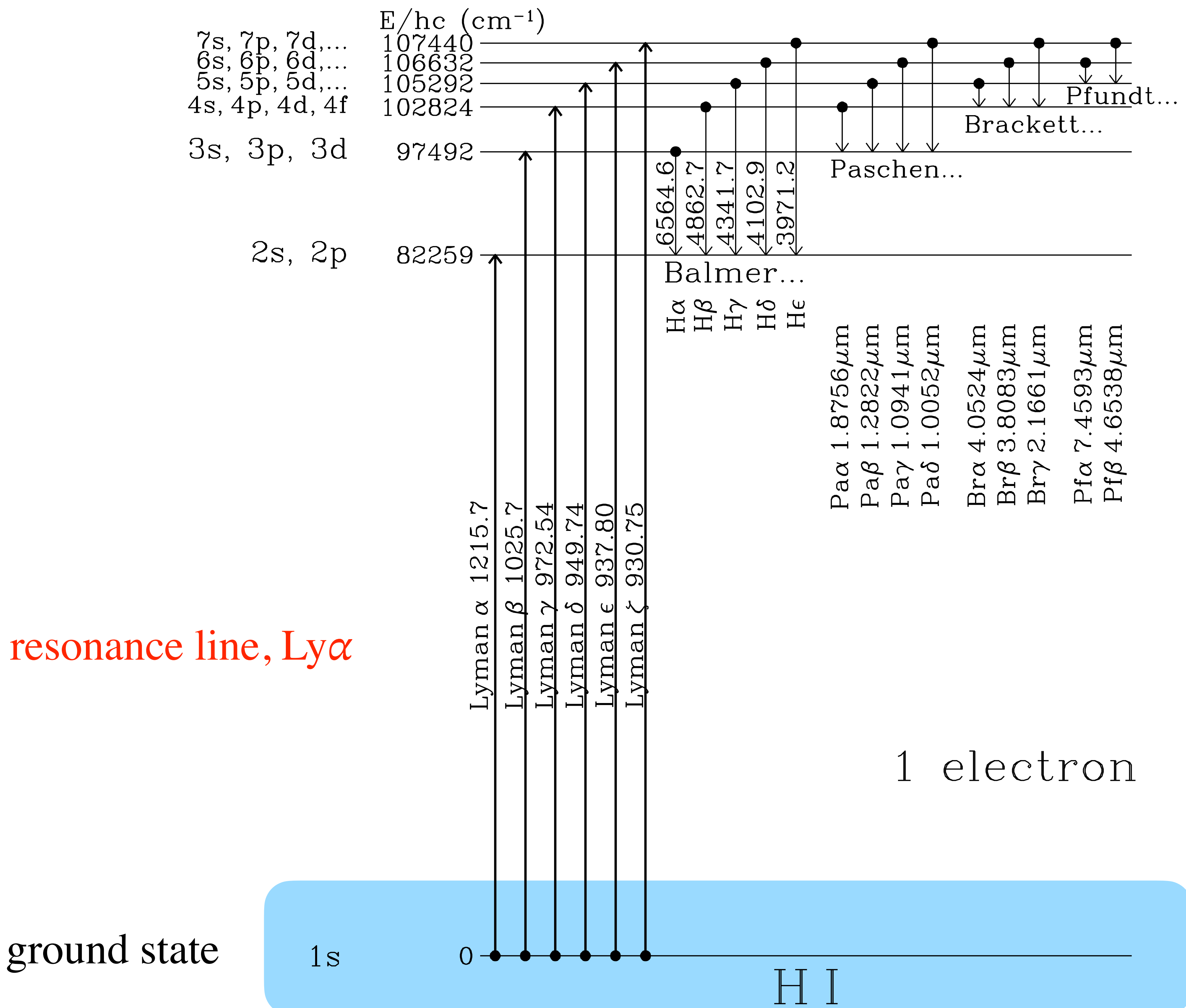
	Element	I→II	II→III	III→IV	IV→V	V→VI	VI→VII	VII→VIII
1	H	13.5984						
2	He	24.5874	54.416					
3	Li	5.3917	75.640	122.454				
4	Be	9.3227	18.211	153.894	217.719			
5	B	8.2980	25.155	37.931	259.375	340.226		
6	C	11.2603	24.383	47.888	64.494	392.089	489.993	
7	N	14.5341	29.601	47.449	77.474	97.890	552.072	667.046
8	O	13.6181	35.121	54.936	77.414	113.899	138.120	739.293
9	F	17.4228	34.971	62.708	87.140	114.243	147.163	185.189
10	Ne	21.5645	40.963	63.423	97.117	126.247	154.214	207.271
11	Na	5.1391	47.286	71.620	98.91	138.40	172.183	208.50
12	Mg	7.6462	15.035	80.144	109.265	141.270	186.76	225.02
13	Al	5.9858	18.829	28.448	119.992	153.825	190.477	241.76
14	Si	8.1517	16.346	33.493	45.142	166.767	205.267	246.481
15	P	10.4867	19.769	30.203	51.444	65.025	220.422	263.57
16	S	10.3600	23.338	34.790	47.222	72.594	88.053	280.948
17	Cl	12.9676	23.814	39.911	53.465	67.819	97.030	114.201
18	Ar	15.7596	27.630	40.735	59.686	75.134	91.00	124.328
19	K	4.3407	31.628	45.806	60.913	82.66	99.4	117.6
20	Ca	6.1132	11.872	50.913	67.27	84.51	108.8	127.2
21	Sc	6.5615	12.800	24.757	73.489	91.69	110.7	138.0
22	Ti	6.8281	13.576	24.492	43.267	123.7	119.533	140.846
23	V	6.7462	14.655	29.311	46.709	65.282	128.125	150.641
24	Cr	6.7665	16.486	30.959	49.160	69.456	90.635	160.175
25	Mn	7.4340	15.640	33.668	51.2	72.4	95.60	119.203
26	Fe	7.9024	16.188	30.651	54.801	75.010	99.063	124.976
27	Co	7.8810	17.084	33.50	51.27	79.5	102.	129.
28	Ni	7.6398	18.169	35.187	54.925	76.06	107.87	133.
29	Cu	7.7264	20.292	36.841	57.380	79.846	103.031	138.862
30	Zn	9.3492	17.964	39.723	59.573	82.574	133.903	133.903

Notes:

- Ionization potentials from Ralchenko et al. (2010)
- The light line separates ions with $I < I_{\rm He}$ from ions with $I > I_{\rm He} = 24.6\,{\rm eV}$.
- Ions to right of the heavy line (with $I > I_{\rm He\,II} = 54.4\,{\rm eV}$) are not abundant in gas photoionized by O or B stars and are therefore indicative of photoionization by WR stars, PN nuclei, or collisional ionization in shocked gas.

Energy Level Diagrams

- 1 electron



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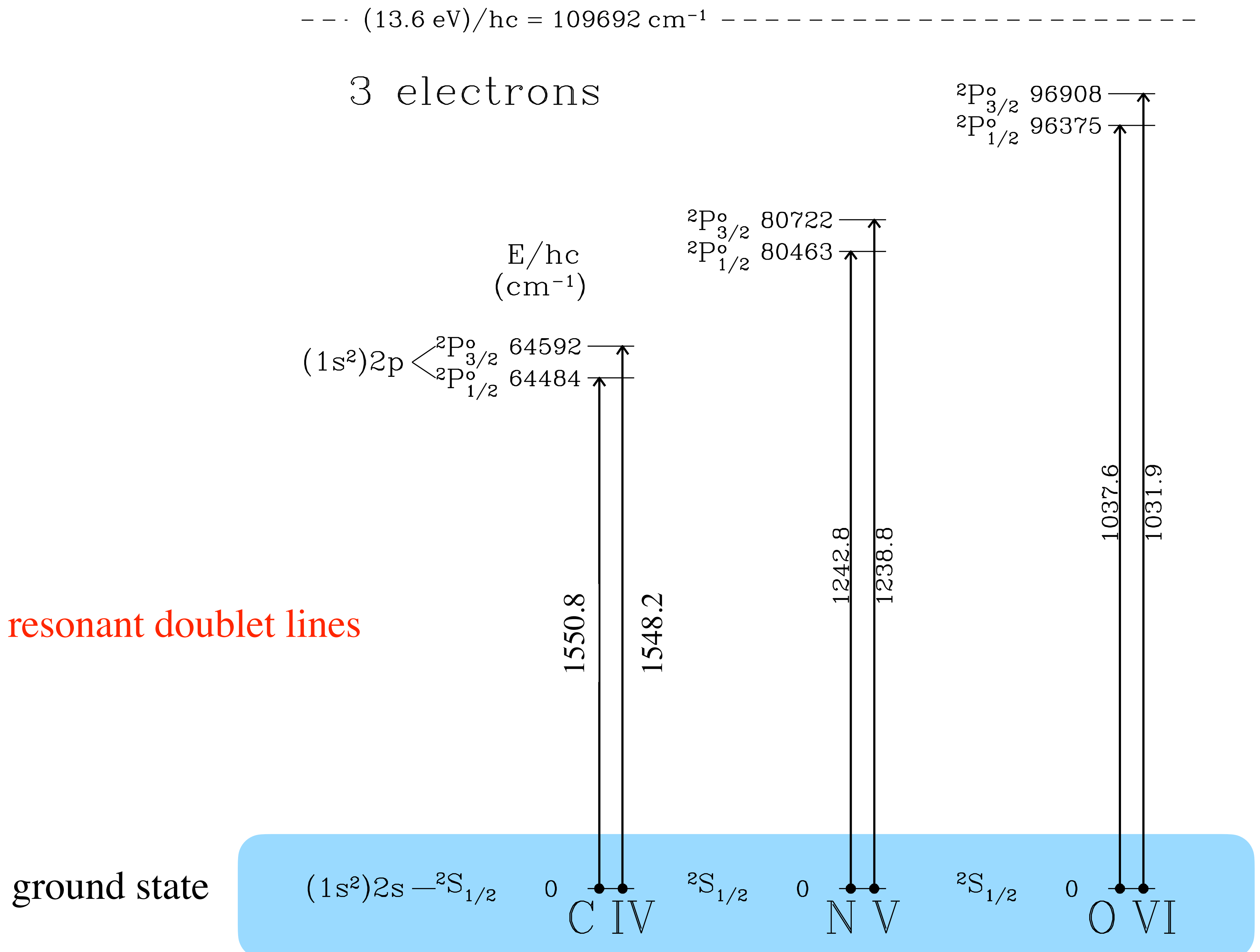
- 3 electrons (Lithium-like ions)



[Draine] Physics of the Interstellar and Intergalactic Medium